Isobutyl nitrite

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 8.65

Global applicability domain: Inside

Local applicability domain index: 4.23e-01

Confidence level: 8.04e-01

Nearest Neighbors from the Training Set

Image not found
2-Butanone oxime
Measured: 5.01
Predicted: 5.34

Image not found
Furan
Measured: 5.01
Predicted: 4.88

Image not found
Piperidine, 1-methyl-
Measured: 4.47
Predicted: 5.88

Image not found
Cyclohexane
Measured: 83.2
Predicted: 59.1

Image not found
2-Nitropropane
Measured: 8.32
Predicted: 7.41